Canonical approach to finite density QCD simulations

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with
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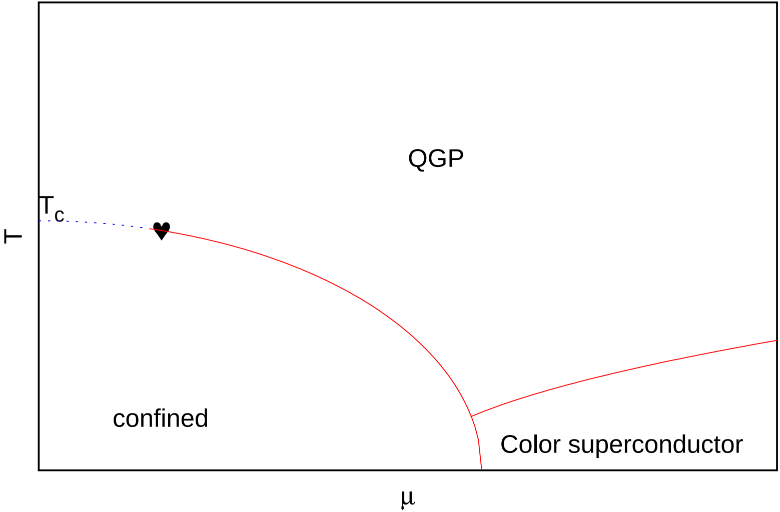
hep-lat/0602024

Phase diagram



To be checked by lattice QCD simulations

The difficulty: “sign” problem

- γ_5-hermiticity:

$$\gamma_5(i\not{p}+m)\gamma_5 = (-i\not{p}+m) = (i\not{p}+m)^\dagger$$

BUT $\gamma_5(i\not{p}+m+\mu\gamma_0)\gamma_5 = (-i\not{p}+m-\mu\gamma_0) = (i\not{p}+m-\mu^*\gamma_0)^\dagger$

$$\boxed{\det \not{D}(\mu) = \det{}^* \not{D}(-\mu^*)}$$

det complex unless $\mu = 0$ (or $i\mu_I$)

- Corollary: measure ϖ must be complex

$$\langle \mathrm{Tr\ Polyakov} \rangle = \exp(-\tfrac{1}{T}F_q) = \langle \mathrm{Re\ Pol} \times \mathrm{Re}\varpi - \mathrm{Im\ Pol} \times \mathrm{Im}\varpi \rangle$$
$$\langle \mathrm{Tr\ Polyakov}^* \rangle = \exp(-\tfrac{1}{T}F_{\bar{q}}) = \langle \mathrm{Re\ Pol} \times \mathrm{Re}\varpi + \mathrm{Im\ Pol} \times \mathrm{Im}\varpi \rangle$$
$$F_q \neq F_{\bar{q}} \Rightarrow \mathrm{Im}\varpi \neq 0$$

- $Z(\mu) = \int \mathcal{D}U\, e^{-S_g}\, \det{}^{N_f} \not{D}(\mu) \quad \rightarrow$ no Monte Carlo

$Z_{MC} = \ldots |\det|$ or $\det(\mu = 0)$ or ...

All Monte Carlo ensembles have zero *average* baryon density: $\langle \rho \rangle = 0$

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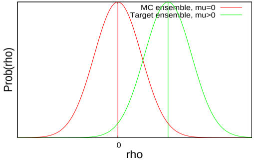
Two problems: sign and overlap

MC ensemble has zero *average* baryon density ρ ⇒ exploit fluctuations in ρ



Each MC config has complex weight in target ensemble: sign problem.
⟶ noisy results

Larger volume.
Overlap problem becomes clear, starting with large-ρ tail
⟶ wrong results (Glasgow method)

Canonical: no large-ρ tail ⇒
reduced overlap pb. ⟶ more reliable
Same thermodynamic limit

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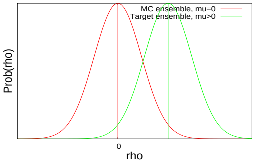

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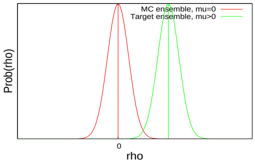

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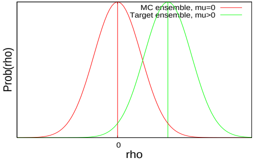

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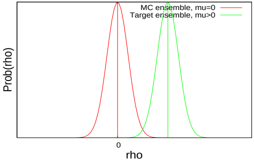

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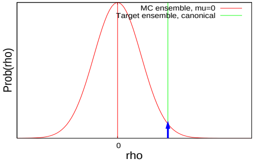

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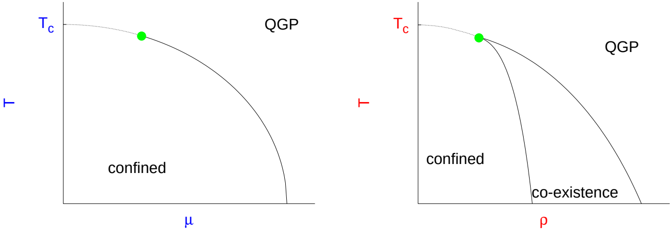
Additional features

- Baryon number B fixed during Heavy-Ion collision
- Canonical simulations have different systematic errors

Hasenfratz & Toussaint; Alford et al.; PdF & Kratochvila; Alexandru et al.

- Phase diagram: $(T, \mu) \longrightarrow (T, \rho)$



Grand canonical Canonical

- Fix B (small), increase V, lower T $\longrightarrow$ nuclear interactions

Canonical formalism on the lattice

- Fix baryon number B

$$\rightarrow \delta(3B - \int d^3x\, \bar{\psi}\gamma_0\psi) = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\bar{\mu}_I \exp(-i\bar{\mu}_I(3B - \int d^3x\, \bar{\psi}\gamma_0\psi))$$
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- μ_I-dependency is in $\det M(U, i\mu_I)$ only! $\rightarrow$ variance reduction
- Strategy: sample $Z_{GC}(i\mu_I)$ at some fixed $\mu_I = \mu_{I_0}$
  Fourier transform each determinant exactly $\rightarrow$ work $\sim L_s^9 \times L_t$
  $\det(U, i\mu_I) = \sum_{-3V}^{+3V} c_q(U)\, \exp(iq\frac{\mu_I}{T})$ Hasenfratz & Toussaint

$$\frac{Z_C(B=\frac{q}{3})}{Z_{GC}(i\mu_{I_0})} = \langle \frac{1}{\det(U, i\mu_{I_0})} c_q(U) \rangle$$

- Combine many ensembles with Ferrenberg-Swendsen

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From canonical to grand canonical

Version 1: Fugacity Expansion: $\mu \longrightarrow B$

$$\langle B(\mu)\rangle = \frac{\sum_{B=-V}^{V} B\, Z_C(B) e^{B\frac{3\mu}{T}}}{\sum_{B=-V}^{V} Z_C(B) e^{B\frac{3\mu}{T}}}$$

Version 2: Saddle Point Approximation: $B \longrightarrow \mu \qquad (\rho \equiv \frac{B}{V})$

$$Z_{GC}(\mu) = \int d\rho\, e^{-\frac{V}{T}(f(\rho)-3\mu\rho)}$$

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Setup: 6^3x4, $a \sim 0.3$ fm, $N_f = 4$ staggered fermions, $m_\pi \sim 350$ MeV

$\Rightarrow$ 1rst-order transition expected for all μ

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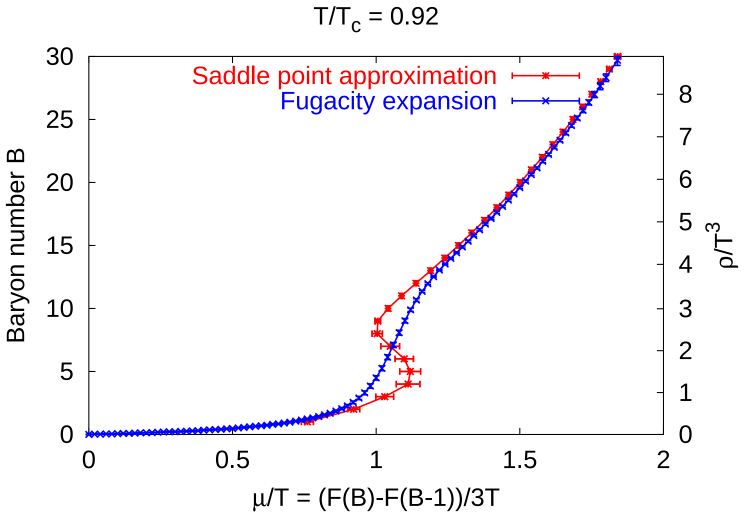
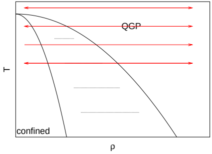
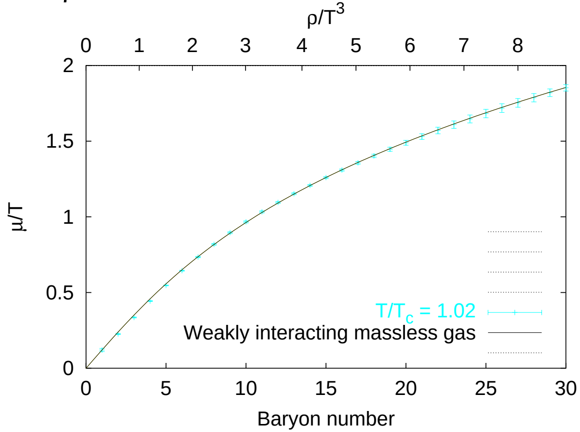

T/T_c = 0.92
Saddle point approximation
Fugacity expansion
Baryon number B
ρ/T^3
μ/T = (F(B)-F(B-1))/3T
0
0.5
1
1.5
2
0
5
10
15
20
25
30
0
1
2
3
4
5
6
7
8

$\frac{\mu(B)}{T} = \frac{F(B)-F(B-1)}{3T}$

Flip coordinates: μ versus ρ

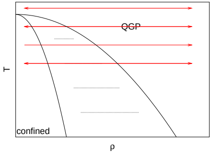


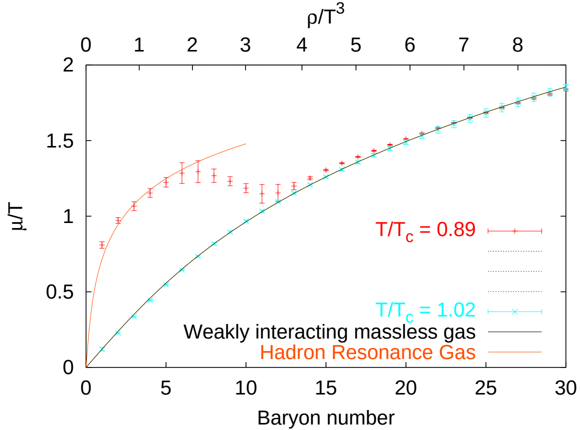


$\frac{\rho(\mu)}{T^3} \approx 2b_2 c_2^{SB}\left(\frac{\mu}{T}\right) + 4b_4 c_4^{SB}\left(\frac{\mu}{T}\right)^3 \rightarrow b_2 = 0.92(1), b_4 = 2.18(1)$

Little departure from free gas

Low density phase consistent with Hadron Resonance Gas





$$\frac{\rho(\mu)}{T^3} = 3F(T)\sinh\frac{3\mu}{T} \rightarrow F(T) = 0.048(3)$$

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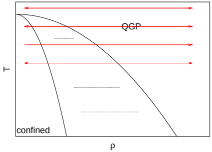
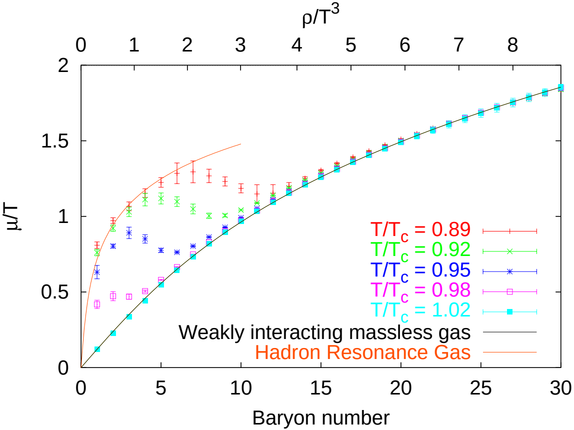
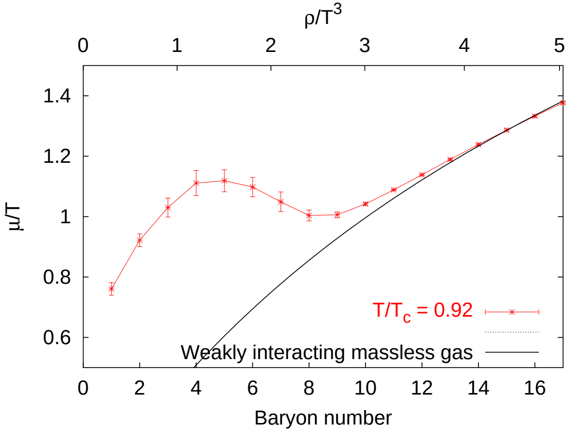




Good accuracy up to $\frac{\mu}{T} \sim 2$, 30 baryons

Fluctuations in transition region physical

Maxwell Construction



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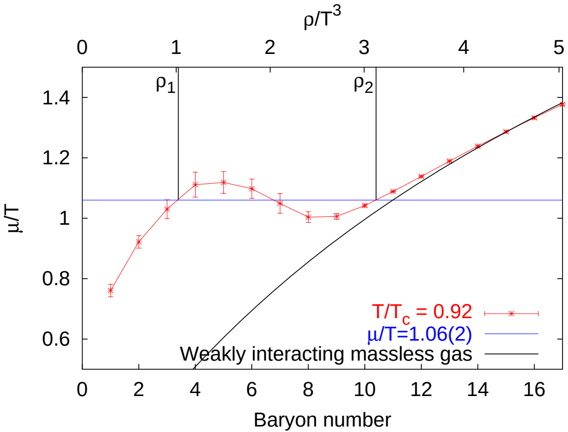
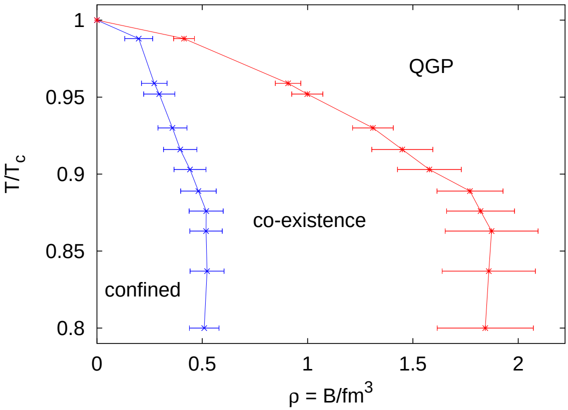


$$\frac{1}{T}\int_{\rho_1}^{\rho_2} d\rho\left(f'(\rho)-\mu\right)=0 \longrightarrow f(\rho_1)-\mu\rho_1=f(\rho_2)-\mu\rho_2$$

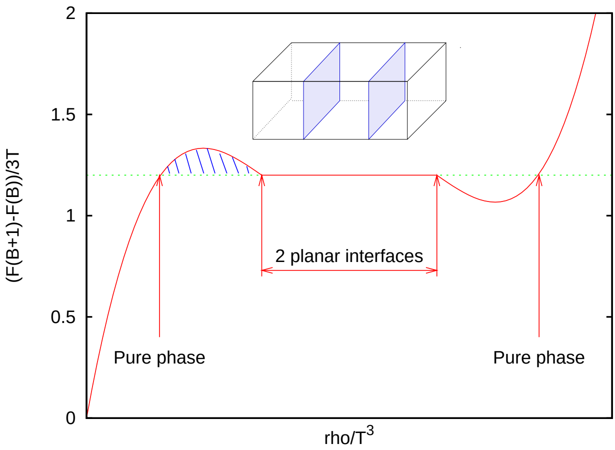
ie. phase transition

Phase Diagram $T - \rho$



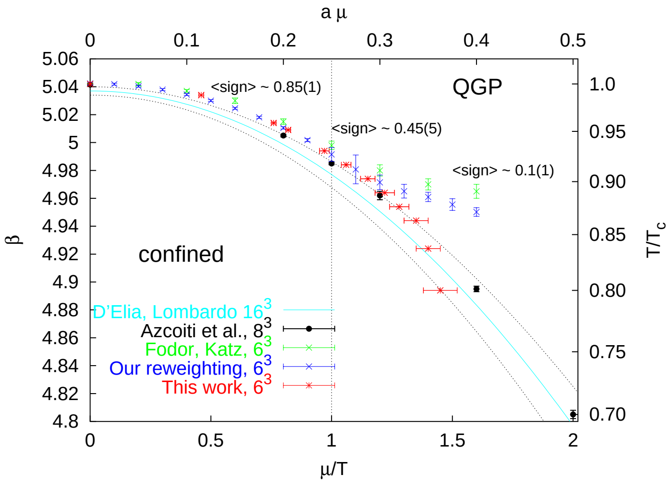
Compare ρ_1 with nuclear density $0.17/\mathrm{fm}^3$

Interface tension



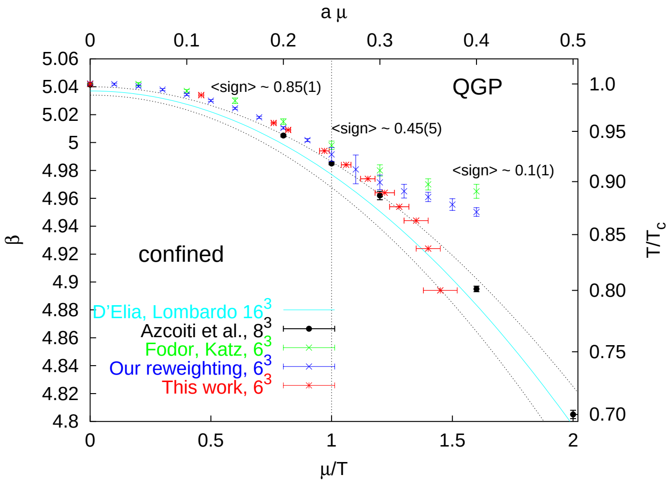
Shaded area = free energy of two L^2/T interfaces $\longrightarrow \sqrt{\frac{\sigma}{T}} \sim 35 - 45$ MeV

Phase Diagram $T - \mu$: comparing apples with apples



i) reweighting becomes unreliable

Phase Diagram $T-\mu$: comparing apples with apples



ii) systematic error of analytic continuation not studied at $\frac{\mu}{T} > 1$

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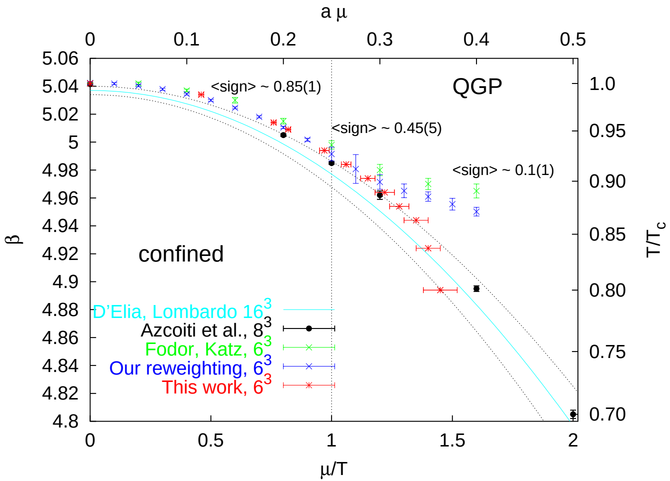


iii) $\beta_c(a\,\mu)$ must bend down to match expectations at $\beta = 0$

Conclusions

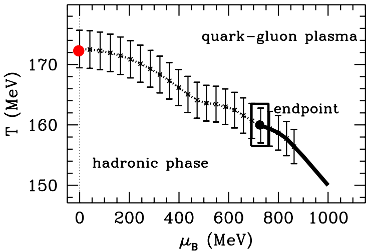
- Lattice QCD at finite μ not for the timid
- Time has come to assess systematic errors: compare methods
- Phase boundary under control for $\mu/T \lesssim 1$:
  continuum, chiral extrapolations ?
- **Canonical formalism:**
  - different systematics
  - overlap problem less severe $\longrightarrow$ more reliable
  - prospect: study ab initio nuclear interactions

Numerical approaches

I. Reweighting in (μ, β) from $(\mu = 0, \beta_c)$

Fodor & Katz

$$Z(\mu,\beta) = \langle \frac{\exp(-\beta S_g)\det M(\mu)}{\exp(-\beta_c S_g)\det M(\mu{=}0)} \rangle Z_{MC}(\mu{=}0,\beta_c)$$



Statistical errors under control ? Overlap problem

Numerical approaches

I. Reweighting in (μ, β) from $(\mu = 0, \beta_c)$

Fodor & Katz

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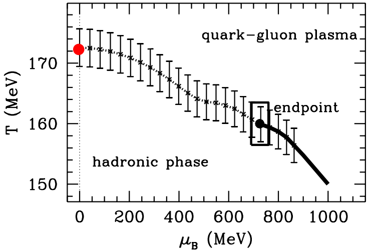

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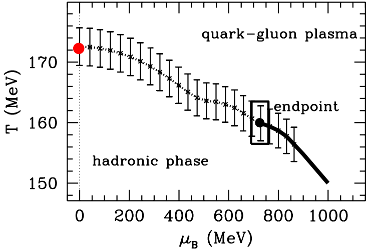

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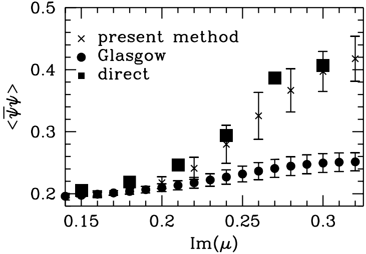

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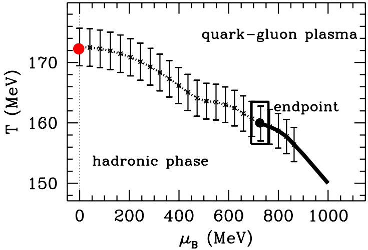

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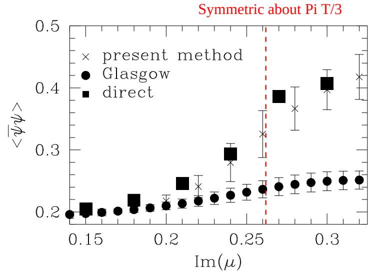

Aside: phase diagram for imaginary μ

- Symmetries:
  - $Z(+\mu) = Z(-\mu)$ even
  - $Z(\mu + i\frac{2\pi T}{3}k) = Z(\mu)$ periodic
- Phase diagram:

$\Longrightarrow$ Z_3 transition at $\mu_I = \frac{\pi}{3}T$, ie. $amu_I = \frac{\pi}{3N_t}$

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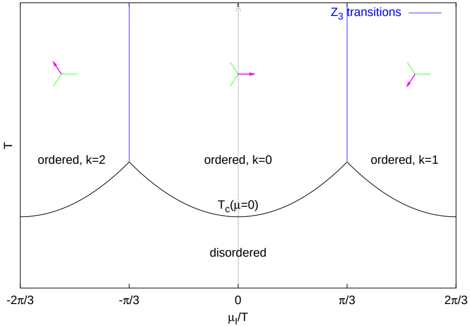

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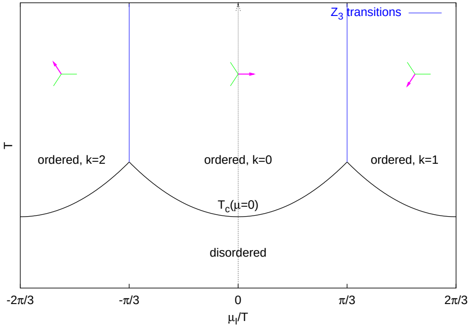

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MILC, .., TARO, Bielefeld-Swansea II, Gavai & Gupta

A few derivatives (max. 4); convergence?

Choose m_q, look for non-analyticity at critical point ?

III. Imaginary μ + analytic continuation

PdF & OP, D'Elia & Lombardo, Giudice & Papa, Chen & Luo, Azcoiti et al.

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Fit with truncated Taylor series, then change $\mu^2 \rightarrow -\mu^2$

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Phase diagram vs $(m_{u,d}, m_s)$, T and μ

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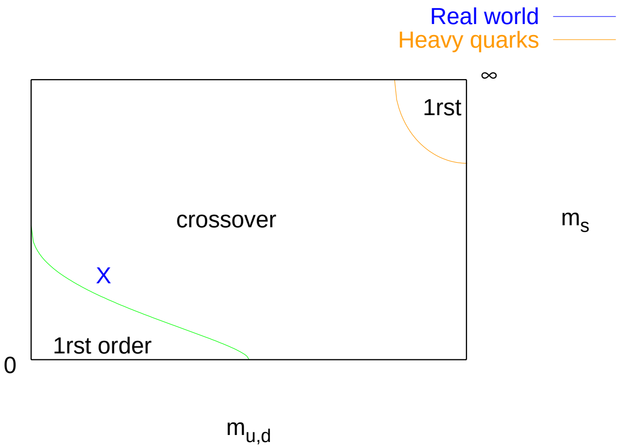

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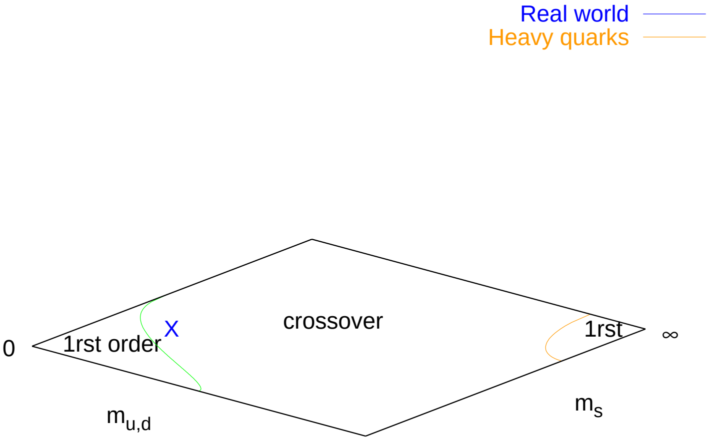

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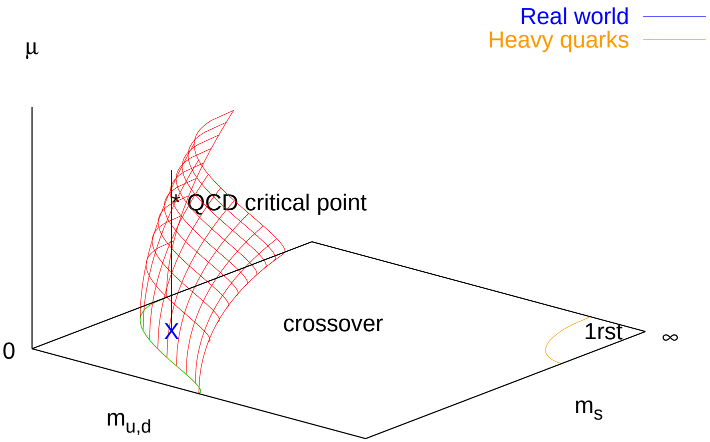

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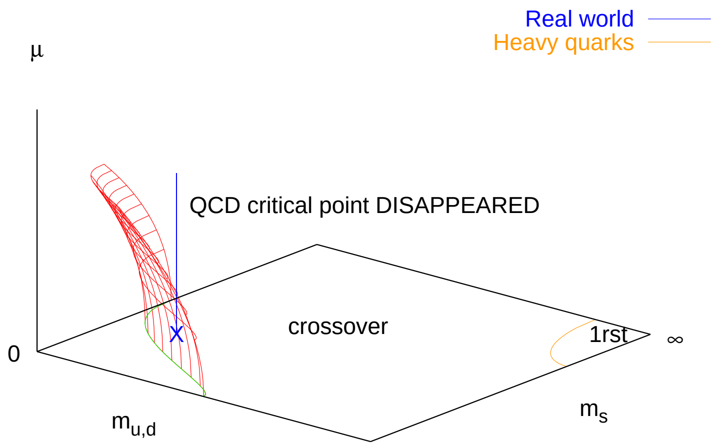

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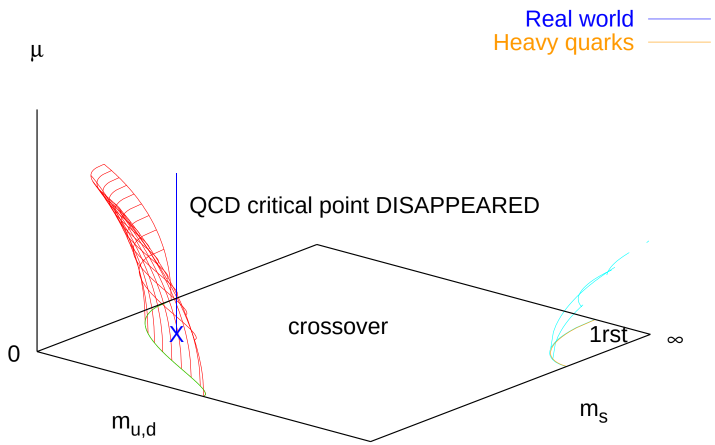

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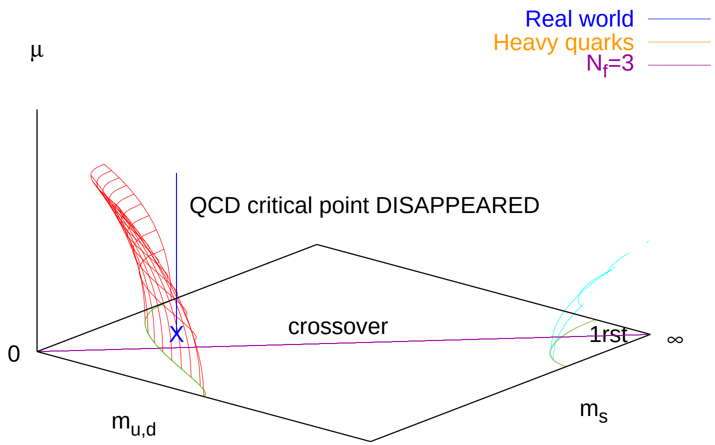

Strong coupling limit?